

Critical decay exponent of the pair contact process with diffusion

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We study the pair contact process with diffusion (PCPD) by extensive Monte Carlo simulations, focusing on the density decay exponent δ at criticality. Studying how the ratio of the density and the pair density behaves at criticality, we estimate the exponent χ of the leading correction to scaling as $\chi = 0.37 \pm 0.01$. With χ so obtained, we study the effective exponent of the critical density decay, to conclude that $\delta = 0.185 \pm 0.010$ which is different from the critical exponent of the directed percolation (DP), 0.1595.

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I. INTRODUCTION

The pair contact process with diffusion (PCPD) is an interacting particles system with diffusion, pair annihilation ($2A \rightarrow 0$), and creation of particles by a pair ($2A \rightarrow 3A$). A decade-long research has failed to elicit a full consensus concerning the universality class of the one dimensional PCPD (for a review of the early controversy, see Ref. [1]). Two competing hypotheses are struggling for survival; does the PCPD belong to the directed percolation (DP) universality class [2–4], or not [5–7]?

The only consensus is that the PCPD has very strong corrections to scaling, which is the reason why reported numerical values of the critical exponents are widely scattered [2–13]. To overcome the strong corrections to scaling, a few approaches have been put forward. In Ref. [5], it was suggested that the so-called ‘soft-core boson’ PCPD model does not have such strong corrections and that the PCPD does not belong to the DP class. However, it turned out that the ‘soft-core boson’ model actually has strong corrections to scaling [3]. Besides, the suggested exponent in Ref. [5] was disputed [3].

Rather than facing with the strong corrections to scaling, Park and Park suggested indirect tests about the universality class in a series of papers [6, 7, 14, 15]. When relative motion of particles and pairs is spatially biased, a completely different critical behavior from the DP as well as from the PCPD appears [6, 14]. Since this critical change due to a spatial bias has not been observed in models known to belong to the DP class, this was argued to be the evidence that the PCPD does not belong to the DP class [6]. When an interaction which clearly makes the system belong to the DP class is introduced to the PCPD, nontrivial crossover behaviors have emerged [7, 15]. Quite interestingly, a nontrivial crossover was observed between two models belonging to the DP class [16]. On one hand, this nontrivial crossover in the DP class is mediated by the drastic shrink of the number of absorbing states (from infinity to one, so to speak). On the other hand, the crossover from the PCPD

to the DP has nothing to do with the structural change of the absorbing space. Since the ‘crossover’ between DP models without structural change of absorbing space is mostly trivial (no exception has ever been reported), it is again claimed that the PCPD does not share critical behavior with the DP [7, 15].

Admittedly, however, the indirect tests cannot fully answer the question. Thus, we feel it necessary to study the PCPD extensively to find the critical exponent directly. Although the strong corrections to scaling is a difficult obstacle hard to evade, it can be helpful if we know how strong the corrections are. In this paper, we carefully study the corrections to scaling. Then, using the information about the corrections to scaling, we will estimate the critical decay exponent.

The paper is organized as follows: After introducing the model in Sec. II, we analyze simulation results in Sec. III. In Sec. IV, we discuss about our analysis and summarize our work.

II. MODEL

The model we are interested in is the one-dimensional parity-conserving pair contact process with diffusion first introduced in Ref. [17]. Since the parity conservation does not play any role in determining the universality class [15, 17], we will simply refer to this model as the PCPD. The model is defined on a one-dimensional lattice of size L with periodic boundary conditions. The state at each site is either occupied by a particle (A) or empty (\emptyset); every site can accommodate at most one particle. The dynamics can be defined as

$$\begin{aligned} A\emptyset &\xleftrightarrow{1/2} \emptyset A, & AA &\xrightarrow{p} \emptyset\emptyset, \\ AA\emptyset\emptyset &\xrightarrow{\sigma} AAAA, & \emptyset\emptyset AA &\xrightarrow{\sigma} AAAA, \end{aligned} \quad (1)$$

where $\sigma = (1-p)/2$. The process starts from the fully occupied initial condition. Obviously, a configuration without a particle is an absorbing state. Although a configuration with a single particle is not an absorbing state in a strict sense, we loosely define such a state as absorbing because a single particle alone in the system cannot

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increase the number of particles. The PCPD in the conventional setting ($2A \rightarrow 0$, $2A \rightarrow 3A$) also has such two ‘absorbing’ states.

In simulations, we keep a list of the position of every particle for all time. Assume that there are N_t particles at time t . Among N_t particles, we choose one with equal probability. Let us assume that the chosen particle is located at site i . With probability $\frac{1}{2}$, one of two nearest neighbors of site i is chosen. Let us call the index of the chosen site j (j is either $i+1$ or $i-1$; recall that we are using periodic boundary conditions). If site j is empty, the particle at site i moves to site j . If site j is also occupied, two particles at both sites (i and j) are annihilated with probability p . But with probability $1-p$, the pair will try to branch another two particles. If a branching event is scheduled, we choose one of two directions with equal probability. If the direction is determined, we check if two nearest sites of the pair along the chosen direction are both empty. If so, two new particles are placed there, but otherwise nothing happens and there is no change of configuration. After the attempt, time increases by $1/N_t$ and the list is appropriately updated.

During simulations, we measured the (particle) density $\rho(t)$ and the pair density $\rho_p(t)$ which are defined as

$$\rho(t) = \frac{1}{L} \sum_i \langle s_i(t) \rangle, \quad \rho_p(t) = \frac{1}{L} \sum_i \langle s_i(t) s_{i+1}(t) \rangle, \quad (2)$$

where $s_i(t)$ is a random variable which takes 1 (0) if site i is occupied (vacant) and $\langle \dots \rangle$ means the average over ensembles. We also counted the number of runs which fall into one of the absorbing states, but all simulation results to be reported later did not end up with an absorbing state up to the observation time.

III. CRITICAL DECAY EXPONENT

At criticality, the density is expected to show power-law behavior with corrections to scaling such as

$$\rho(t) \sim a_1 t^{-\delta} (1 + c_1 t^{-\chi}), \quad (3)$$

where δ is the critical decay exponent, χ is the exponent of the leading correction, and a_1, c_1 are (nonuniversal) constants. For the DP class, $\delta \approx 0.1595$ in one dimension. Since the two dimensions are believed to be the upper critical dimensions of the PCPD, we assume that there is no logarithmic correction in the one dimensional system.

To determine the critical exponent δ from numerical data, it is customary to analyze the effective exponent defined as

$$-\delta_{\text{eff}}(t; b) = \frac{\ln \rho(t) - \ln \rho(t/b)}{\ln b}, \quad (4)$$

where b is a time independent constant. At criticality the asymptotic behavior of the effective exponent should be

$$-\delta_{\text{eff}}(t; b) = -\delta - c_1 \frac{b^\chi - 1}{\ln b} t^{-\chi} + o(t^{-\chi}). \quad (5)$$

Thus, if we plot the effective exponents $-\delta_{\text{eff}}$ as a function of $t^{-\chi}$ at criticality, the curve should approach to the critical exponent with finite slope as $t^{-\chi} \rightarrow 0$. On the other hand, if the system is in the active (absorbing) phase near the critical point, the effective exponent eventually veers up (down) as $t^{-\chi} \rightarrow 0$. The information about χ , therefore, will be very useful to find the accurate value of the critical exponent.

To find χ without prior knowledge of δ , we need another quantity which decays as $t^{-\delta}$ in the asymptotic limit. A natural candidate is the pair density $\rho_p(t)$. Although a mean field theory and simulations of higher-dimensional model [18] as well as the one dimensional driven PCPD [6] have shown that the pair density does not necessarily follow the same power law behavior as the density, numerical studies of the one-dimension PCPD (for example, see Ref. [2, 7]) show that $\rho(t)/\rho_p(t)$ indeed approaches to a finite number as $t \rightarrow \infty$ at criticality. Hence, it is expected up to the leading correction that

$$\rho_p(t) \sim a_2 t^{-\delta} (1 + c_2 t^{-\chi}), \quad (6)$$

where a_2 and c_2 are constants. Assuming $c_1 \neq c_2$, the ratio of $\rho(t)$ and $\rho_p(t)$ at the critical point can be expanded as

$$R(t) \equiv \frac{\rho(t)}{\rho_p(t)} \sim \frac{a_1}{a_2} [1 + (c_1 - c_2) t^{-\chi} (1 + C t^{-\chi})], \quad (7)$$

where we have assumed that the next leading correction to scaling is not larger than $t^{-2\chi}$ and $C \neq 0$. This ratio has already been studied in Refs. [2, 4] and, albeit in a different context, in Ref. [7]. Note that two assumptions have been employed to arrive at Eq. (7). The plausibility of these two assumptions will be discussed in Sec. IV.

Since δ does not appear in $R(t)$, we can study χ directly using the effective exponent

$$\chi_{\text{eff}}(t; b) \equiv \ln \left(\frac{R(t/b) - R(t/b^2)}{R(t) - R(t/b)} \right) / \ln b, \quad (8)$$

where b is a time-independent constant. From Eq. (7), the asymptotic behavior of $\chi_{\text{eff}}(t)$ at criticality is expected to be

$$\chi_{\text{eff}}(t; b) \sim \chi + C \frac{b^{2\chi} - 1}{\ln b} t^{-\chi}. \quad (9)$$

Now we need the critical point. Actually, the critical point of the model in question is quite accurately estimated in Ref. [15], which was the reason why we study the present model rather than the conventional one.

Equipped with Eq. (9) together with the accurately estimated critical point, we will find χ by the Monte Carlo simulations. To this end, we simulated the system with $L = 2^{19}$ for several p 's around the critical point (from 0.180 210 to 0.180 215) up to $t = 10^7$. Since there is no significant difference among these simulations up to $t = 10^7$, we will only present the results for $p = 0.180 214$ which later will be asserted to be the critical point. Because we have to remove the leading behavior of $R(t)$,

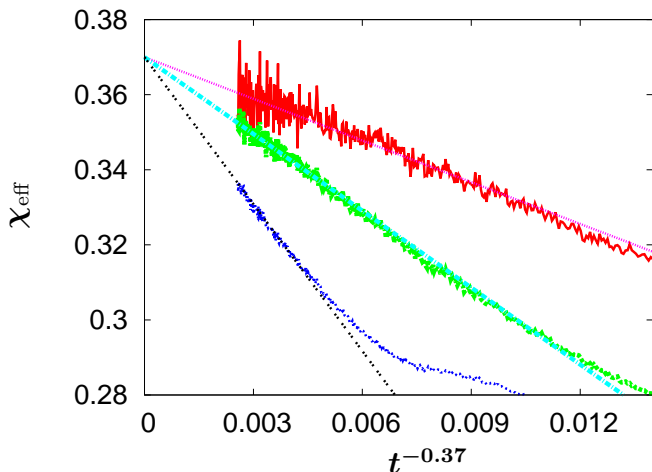


FIG. 1. (Color online) Plots of $\chi_{\text{eff}}(t; b)$ for $b = 10^{3/2}$ (upper curve), 10^2 (middle curve), and $10^{5/2}$ (lower curve) as a function of $t^{-0.37}$. The straight lines are resulting fitting functions which were found as explained in the text.

statistical noise could be enormous unless the number of ensembles is large enough. To reduce statistical noise, we collected data from 25 000 ensembles. Then, the effective exponents are calculated using $b = 10^{3/2}$, 10^2 , and $10^{5/2}$.

To extract χ from χ_{eff} , we first analyzed $\chi_{\text{eff}}(t; b = 10^{5/2})$ which is least noisy among three effective exponents. For a given χ , we fit $\chi_{\text{eff}}(t; 10^{5/2})$ using Eq. (9) with C to be a fitting parameter. We set the fitting range to be from $t = 2 \times 10^6$ to 10^7 . Then, we graphically checked if Eq. (9) can fit the other effective exponents when the same C for given χ is used. The best fit is attained when $\chi = 0.37$ is used; see Fig. 1. In this case, C is estimated as $\simeq 2.15$. Since $\chi = 0.36$ or 0.38 does not yield a nice fitting (see Supplemental Material at [URL] for the fitting results when $\chi = 0.36$ and 0.38 are used), we estimated χ as $0.37(1)$ with the number in parentheses to indicate the error. Note that this estimation of χ is consistent with the previous studies [2, 4]. In a sense, the leading correction to scaling is not terrifyingly huge; for $t = 10^8$, the leading correction is of the order of 10^{-3} . Hence, with the present computing power, it seems feasible to find the critical exponent of the PCPD.

Now we will move on to the analysis of the effective exponent δ_{eff} using $\chi = 0.37$. We present the simulation results for $p = 0.180\ 213$ (300 runs), $0.180\ 214$ (456 runs), and $0.180\ 215$ (300 runs) with larger system size ($L = 2^{21}$) and longer observation time ($t = 10^9$) than above. Up to $t = 10^9$, no simulated system falls into an absorbing state, which minimally guarantees the negligible finite size effect. Actually, all simulated samples always contain at least one pair.

In Fig. 2, the effective exponents calculated with $b = 100$ are plotted as a function of $t^{-\chi}$ for different p 's (see Supplemental Material at [URL] for the pair-density effective exponents plot which looks more or less same as Fig. 2). The data with $p = 0.180\ 213$ ($0.180\ 215$) veers up

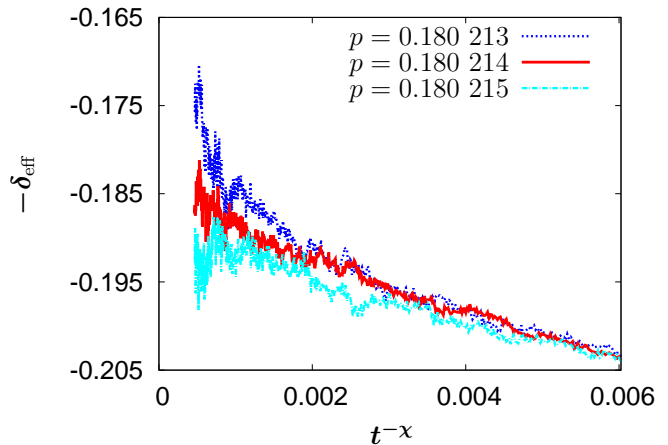


FIG. 2. (Color online) Plots of $-\delta_{\text{eff}}$ using $b = 100$ as a function of $t^{-\chi}$ with $\chi = 0.37$ for $p = 0.180\ 213$ (upper curve), $0.180\ 214$ (middle curve), and $0.180\ 215$ (lower curve).

(down), which signals that the system is in the active (absorbing) phase. In fact, the curvature for $p = 0.180\ 215$ is not so conspicuous, but if we use $b = 10$, one can see a clear curvature for this case (see Supplemental Material at [URL] for the behavior of effective exponents calculated with $b = 10$). Since the data with $p = 0.180\ 214$ approaches the ordinate with finite slope, we conclude that $p_c = 0.180\ 214(1)$ and $\delta = 0.185(10)$. Our estimation of δ should be compared with that of the DP class, 0.1595 . Quite interestingly, the critical decay exponent we found in this paper is close to the upper limit of δ set by Hinrichsen [3].

IV. SUMMARY AND DISCUSSION

To summarize, we studied the pair contact process with diffusion with modulo 2 conservation. At first, we systematically measured the leading correction to scaling described by the exponent χ . Then, by the analysis of the effective exponent δ_{eff} along with the estimated χ , we concluded that the critical density decay exponent is $0.185(10)$, which is not compatible with that of the DP class.

When we derive Eq. (9), however, we had to resort to a few assumptions. First, we assume that the coefficients of the leading corrections to scaling of the density and the pair density are different ($c_1 \neq c_2$). Second (along with the first assumption), the next leading corrections to scaling is not larger than $t^{-2\chi}$. We will discuss about these two assumptions in this section.

The assumption of $c_1 \neq c_2$ is actually not built on a firm ground. We cannot fully exclude the possibility that we actually estimated the exponent of the next leading correction, that is, $c_1 = c_2$. In fact, one can easily come up with two quantities whose coefficients of the leading correction are exactly the same.

To see this, let us begin with writing the equation

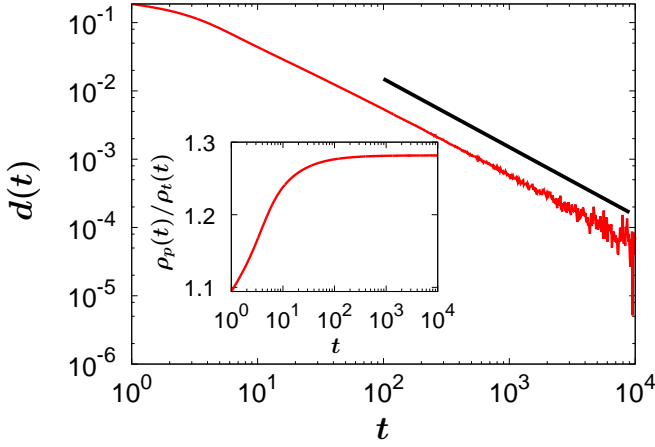


FIG. 3. (Color online) Log-log plot of $d(t) \equiv (1 - p_c)/(1 - 2p_c) - \rho_p(t)/\rho_t(t)$ vs t at $p = p_c$. A straight line segment whose slope is -1 is for the guide to the eyes. Inset: Log-linear plot of $\rho_p(t)/\rho_t(t)$ vs t at $p = p_c$.

about the density behavior in time. A straightforward calculation gives

$$\frac{d}{dt}\rho(t) = 2(1 - 2p)\rho_p(t) - 2(1 - p)\rho_t(t), \quad (10)$$

where $\rho_t(t)$ is defined as

$$\rho_t(t) = \frac{1}{L} \sum_i \langle s_i s_{i+1} [s_{i+2} + (1 - s_{i+2})s_{i+3}] \rangle. \quad (11)$$

We drop the explicit t dependence of s_i for convenience and we have assumed that the system has mirror symmetry; that is, the density of the local configuration $AA\emptyset A$ is assumed to be the same as that of $A\emptyset AA$.

As in Sec. III, let us assume that at the critical point $\rho(t)$ and $\rho_p(t)$ behave in the asymptotic regime as Eqs. (3) and (6), respectively. Since Eq. (10) should be consistent with Eqs. (3) and (6), $\rho_t(t)$ should behave up to the leading correction as

$$\rho_t(t) = a_3 t^{-\delta} (1 + c_3 t^{-\chi}). \quad (12)$$

Since the leading behavior of the time derivative of ρ is $t^{-1-\delta}$, Eq. (10) forces the relation $(1 - 2p_c)a_2 = (1 - p_c)a_3$. By the same token, if $\chi < 1$, c_2 should be equal to c_3 . In fact, any correction larger than t^{-1} should vanish on the right-hand side of Eq. (10). Otherwise, the leading behavior of the term on the left hand side in Eq. (10) which is $t^{-1-\delta}$ cannot be the same as the terms on the right hand side. Hence, if we study the ratio of $\rho_p(t)$ and $\rho_t(t)$, it should approach to the asymptotic value as

$$\frac{\rho_p(t)}{\rho_t(t)} = \frac{1 - p_c}{1 - 2p_c} (1 + et^{-1} + o(t^{-1})), \quad (13)$$

where e is a (nonzero) constant. Hence if we plot

$$d(t) \equiv \frac{1 - p_c}{1 - 2p_c} - \frac{\rho_p(t)}{\rho_t(t)} \quad (14)$$

as a function of t at $p = p_c$, one can see a $1/t$ behavior in the long time limit. In Fig. 3, we depict $d(t)$ vs t in double-logarithmic scales at $p = p_c$ (while we were gathering data for the analysis of χ , we also measured $\rho_t(t)$). As a byproduct, clean $1/t$ behavior of $d(t)$ supports that in Sec. III we studied the regime where $\rho(t)$ and $\rho_p(t)$ are properly described by Eqs. (3) and (6).

As the example of $d(t)$ shows, it is not impossible that the leading correction to scaling in ρ and ρ_p happens to be identical. Although we cannot provide a plausible argument, however, we think that Fig. 2 combined with Eq. (5) provides a numerical evidence that the leading correction of $R(t)$ is same as that of ρ . Note that similar studies in Refs. [2, 4] also implicitly assume that $R(t)$ indeed contain information about the leading correction to scaling.

Actually, Fig. 1 which shows that Eq. (9) correctly describes the behavior of the effective exponent χ_{eff} at the critical point also supports the assumption $c_1 \neq c_2$. To see why, we will investigate what will be the correct asymptotic behavior of χ_{eff} if $c_1 = c_2$. By this assumption, ρ and ρ_p at criticality should take the form ($\chi_1 < \chi_2 < 1$)

$$\begin{aligned} \rho(t) &= a_1 \{1 + ct^{-\chi_1} + f_1 t^{-\chi_2} + o(t^{-\chi_2})\}, \\ \rho_p(t) &= a_2 \{1 + ct^{-\chi_1} + f_2 t^{-\chi_2} + o(t^{-\chi_2})\}, \end{aligned} \quad (15)$$

which gives

$$\begin{aligned} \frac{a_2}{a_1} R(t) &\approx \frac{1 + ct^{-\chi_1} + f_1 t^{-\chi_2}}{1 + ct^{-\chi_1} + f_2 t^{-\chi_2}} \\ &\approx 1 + (f_1 - f_2)t^{-\chi_2}(1 - ct^{-\chi_1}). \end{aligned} \quad (16)$$

If this is the case, the procedure of finding χ explained in Sec. III would not yield a reasonable conclusion.

We can repeat the above discussion to argue that the next correction to scaling is not stronger than $t^{-2\chi}$. This assumption is also supported by Fig. 1 in a self-consistent way. Hence, two assumptions we made are supported self-consistently by the numerical study and the analysis in Sec. III is legitimate.

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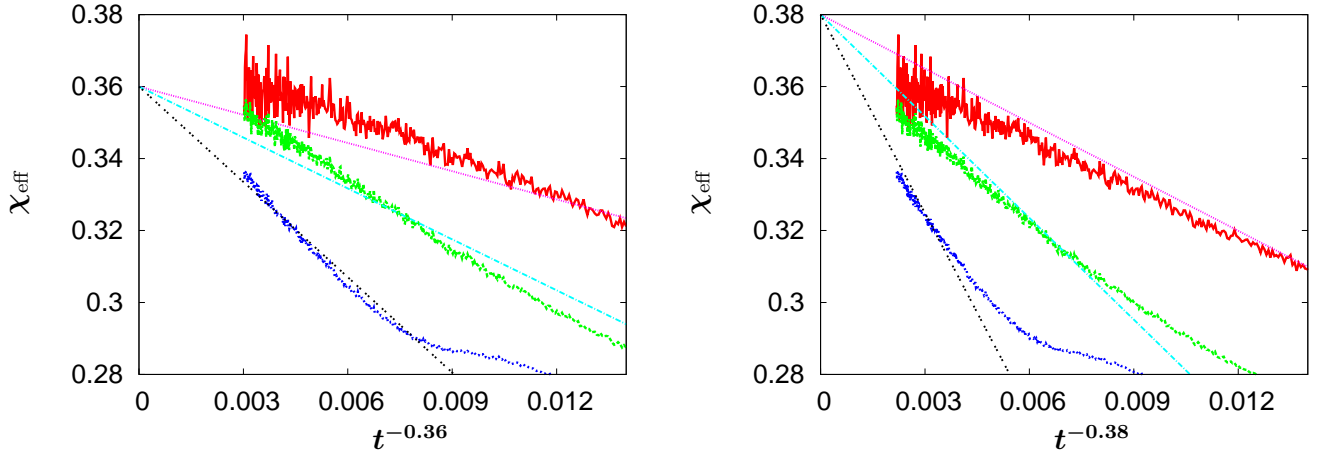
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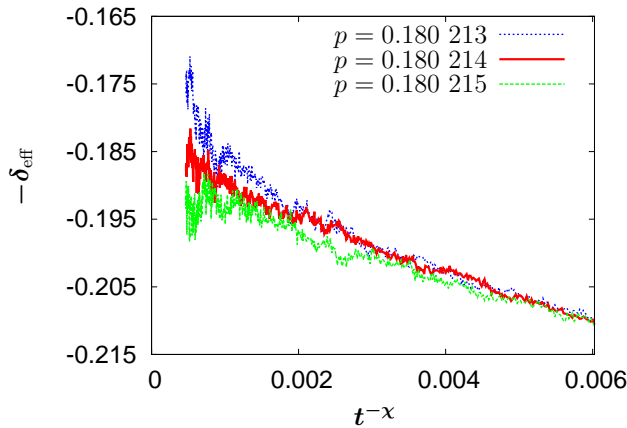
Supplemental Material for “Critical decay exponent of the pair contact process with diffusion”

Su-Chan Park

SM FIG. 1. Fitting results of χ_{eff} using $\chi = 0.36$ (left) and $\chi = 0.38$ (right).



SM FIG. 2. Effective exponent of the pair density with $b = 100$.



SM FIG. 3. Effective exponent of the particle density with $b = 10$.